



Stratospheric age of air computed with trajectories based on various 3-D-Var and 4-D-Var data sets

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Stratospheric age of air computed with trajectories based on various 3-D-Var and 4-D-Var data sets

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Abstract

The age of stratospheric air is computed with a trajectory model, using ECMWF ERA-40 3-D-Var and operational 4-D-Var winds. The sensitivity to the forecast period and assimilation technique are studied, and the results are compared with observations and with results from a chemistry transport model that uses the same data sets. A large number of backward trajectories is started in the stratosphere, and from the fraction of these trajectories that has reached the troposphere, the age of air is computed.

A pilot study in the tropical stratosphere shows that the age increases with increasing length of the forecast series.

Next, for three selected data sets (3-D-Var 1-day and 4-D-Var 3-day forecast series, and 4-D-Var analyses) 5-year backward trajectories are computed that start all over the globe at an altitude of 20 km. For all data sets the computed ages of air in the extratropics are smaller than observed. For 4-D-Var forecast series they are closest to the observations, but still 0.5–1.5 year too small. Compared to the difference in age between the results for the different data sets, the difference in age between the trajectory and the chemistry transport model results is small.

1. Introduction

In a recent study the stratospheric age of air in a chemistry transport model (CTM), driven by different data sets from the European Centre for Medium-Range Weather Forecast (ECMWF), was compared to observations (Meijer et al., submitted, 2004¹). The age of air can be defined as the time that air has resided in the stratosphere after entering it through the tropopause. The results showed that in the extratropics at 20 km altitude the simulated age of air was about twice as small as observed. The

¹Meijer, E., Bregman, B., and van Velthoven, P. F. J.: The influence of data assimilation on the age of air in a global chemistry-transport model, Geophys. Res. Lett., submitted, 2004.

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precise reason for this was not clear. It could be due to the preprocessing involving interpolations that the ECMWF data undergo before they can be used to drive the CTM (Bregman et al., 2003), but also to erroneous stratospheric transport in the original ECMWF data themselves (van Velthoven and Kelder, 1996). In the CTM the vertical velocity is not directly derived from the ECMWF vertical velocity, but instead is computed from the horizontal divergence on the model grid. A mass correction procedure has to be applied to guarantee mass conservation between subsequent meteorological analyses. This part of the preprocessing is known to introduce errors in the vertical velocity. In the ECMWF data errors in the vertical velocity are expected, because the data are not entirely physically consistent. Instead, the assimilation of new observations in the ECMWF model slightly disturbs the physical balance. Although in general this will force the model closer to reality, some quantities that are not observed directly, such as the vertical velocity, might become less realistic. This so-called spin-up problem can be avoided by using data from a general circulation model, which was shown by Schoeberl et al. (2003) to give reasonable estimates of the stratospheric age of air. If data describing the actual state of the atmosphere are needed, then a possible approach to minimize the spin-up problem might be to use forecast series, with a period of a few days, rather than, for example, analyses or first-guess data that are updated every 6 h. With a period of, for example, 3 days, the data will remain physically consistent during 3 days and the perturbation caused by assimilating observations will be seen only once every 3 days, at the transition to a new forecast series. When first-guess (6-h forecast) data are used, such a perturbation occurs every 6 h. On the other hand, the effect of a 3-daily perturbation is not necessarily smaller than that of 12 relatively small 6-h perturbations over 3 days.

The circulation in the ECMWF model has also been shown to depend on the particular model version used (van Velthoven and Kelder, 1996). The ERA-40 data are of special interest because they have been produced with a single model version and therefore inconsistencies due to model updates are absent.

In the present study we investigate the sensitivity of age of air computations, based

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on 3-D winds from the ECMWF model, to the type of forecast series, i.e. the lag between the first forecast time step used and the analysis as well as the length of the forecasts series. We will calculate the age of stratospheric air with the TRAJKS trajectory model (Scheele et al., 1996). Stohl et al. (2001) have shown that the results of the TRAJKS model are consistent with results from two other trajectory models using the same input data. A trajectory model is used rather than a CTM, because the results can then unambiguously be interpreted in terms of the input wind data (Schoeberl et al., 2000). Since in the TRAJKS model the original ECMWF wind data are applied, including the vertical wind on the ECMWF model levels, the possible effect of preprocessing on the results is eliminated.

The study consists of two parts. The first part is a sensitivity study, in which a large number of 50-day-backward trajectories starting in the tropical lower stratosphere is computed. The fraction of the trajectories that has left the stratosphere after this period is a measure for the mean age of the air in the starting region. Since the air in this region is relatively young, the required integration time is relatively short. The 50-day backward trajectories are computed using 9 different ECMWF data sets, including different types of forecasts series and two model versions. In the second part, three of these data sets are selected to compute 5-year backward trajectories that start all over the globe, at an altitude of 20 km, for which the CTM simulations and the observations of the age of air are available. For these longer integrations the mean age of air at the starting points is estimated and compared with the CTM results and with the observations.

2. Method to calculate the age of air

The mean age of air at a specific altitude and latitude in the stratosphere is determined as follows: a large number of 5-year backward trajectories is started at this altitude and latitude, at various longitudes and times. During the 5-year integration we determine daily which fraction of the trajectories has reached the troposphere. The tropopause

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definition used for this will be given below. The fraction of trajectories with an age less than or equal to T , equals the cumulative probability density of T , denoted by $F(T)$. By definition $F(0)=0$ and $F(\infty)=1$. The mean age of air, \bar{T} , is given by

$$\bar{T} = \int_0^{\infty} \frac{dF(T)}{dT} T dT, \quad (1)$$

- 5 where $dF(T)/dT$ is the probability density of T . By using F instead of T as the integration variable, Eq. (1) can be simplified as

$$\bar{T} = \int_0^1 T(F) dF. \quad (2)$$

As will be shown below, after 5 years more than 90% of the trajectories has reached the troposphere. For these trajectories $F(T)$ can be determined from the trajectory results. However, for the remaining trajectories, for which $T > 5$ year, this is not possible. Thus the integral in Eq. (2) can, in first instance, only be computed up to $F \approx 0.9$. However, we found that the long-time tail of the distribution $F(t)$ can be well fitted by an exponentially decaying function, $1 - a \cdot \exp(-bT)$. The values of a and b were computed by fitting this function to the observed values of $F(5 \text{ year})$ and $F(3 \text{ year})$. After this, the integral in Eq. (2) can be estimated up to $F = 1$.

As mentioned above, we need a definition of the tropopause. The results are, however, not particularly sensitive to this choice, as vertical mixing in the troposphere is rapid. Schoeberl et al. (2003) defined the tropopause equatorward of 15° latitude as the level where the potential temperature equals 380 K, and poleward of 15° latitude as the level where the absolute value of the potential vorticity equals $2 \cdot 10^{-6} \text{ Km}^2 \text{ kg}^{-1} \text{ s}^{-1}$. We calculated the pressures of both levels, and used the largest pressure as our definition of the tropopause. This gives a continuously varying tropopause, while the Schoeberl definition can lead to vertical jumps at the transition latitude. To ensure that a trajec-

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tory irreversibly crosses the tropopause, we required that the pressure of the trajectory should remain 10% larger than the tropopause pressure for at least one day.

3. Sensitivity study

In the sensitivity study 50-day backward trajectories are computed for 9 different ECMWF data sets. The main characteristics of the sensitivity experiments are presented in Table 1. The differences between the data sets concern either the year (1997 or 2000), the type of assimilation model (3-D-Var or 4-D-Var model), the length and update frequency of the model forecast (the columns ‘Forecast’ and ‘Update’ are explained below), and the horizontal resolution of the data. All data have a temporal resolution of 6 hours. In experiment 3, e.g. 12, 18, 24 and 30-h forecasts are taken from one base time. As this forecast series has a length of 24 h, it needs to be updated every 24 h. In experiment 6 4-D-Var analyses are applied, hence forecast 0.

The trajectories all start in the tropical stratosphere, at a potential temperature of 460 K, corresponding to an altitude of about 23 km and a pressure of about 50 hPa. The starting points are located at latitudes of 10°S, the equator and 10° N, at 1°-intervals in longitude. The trajectories are started at 12:00 UTC on each of the last 9 days of February. Thus, for each data set 360*3*9=9720 trajectories are computed. At each hour it is determined which fraction of the trajectories has reached the troposphere using the above described procedure.

The fraction of the backward trajectories that has reached the troposphere at or before day 50, to be denoted as $F(50)$, is presented in the rightmost column of Table 1. The first 3 data sets have the same characteristics, except for the type of forecast series. These data sets lead to very different values of $F(50)$, with the largest value, 46%, for the first-guess data, and the smallest value, 15%, for the longest forecast series. Decreasing the horizontal resolution from 1°×1° to 2.5°×2.5° (experiments 3 versus 4) has almost no effect on the value of $F(50)$. Also using a different year from the ERA-40 data set (experiments 4 versus 5) has almost no effect. Remarkably, the value

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of $F(50)$ is further reduced when instead of 3-D-Var data 4-D-Var data are applied. For 4-D-Var analyses (experiment 6) the value of $F(50)$ is 12%, which is smaller than all values computed with any 3-D-Var data set. When using 4-D-Var forecast series with a length of 1 day, 3 days, or 9 days (experiments 7, 8, and 9) the value of $F(50)$ further decreases to 3%. The 3-day and 9-day experiments give the same small value of $F(50)$. In conclusion, the calculations show that the age of air in the tropical lower stratosphere as represented by the different data sets is larger for forecast series than for analyses or first-guess data, and it increases with increasing length of the forecast series. The age for any choice of the operational 4-D-Var data is much larger than for the 3-D-Var data. The decreasing value of $F(50)$, implying increasing age, with increasing length of the forecast series, occurring both in the 3-D-Var and in the 4-D-Var data, indicates that the age of stratospheric air is increased by increasing the physical consistency of the data, i.e. by decreasing the frequency at which forecast series based on different analyses are introduced.

The fraction of the trajectories that has reached the troposphere, as a function of time, is shown in Fig. 1, for the high resolution four 3-D-Var data sets (Exp. 1, 2, 3 and 4), and in Fig. 2 for the 3-D-Var and 4-D-Var year 2000 data sets (experiments 5, 6, 7, 8, and 9). The figures show that longer forecast series generate less vertical transport. Also they show that 4-D-Var generates less transport across the tropopause than 3-D-Var.

Of the different 3-D-Var data sets, the stratospheric transport is probably best described by the one-day forecast series (Table 1, Exp. 3, 4 and 5). Longer 3-D-Var forecast series would probably be even better, but these are not available in the ERA-40 dat set. We will, therefore, use these one-day forecast data in the second part of this study, where we actually calculate the age of air and where 5-year backward trajectories are computed that start in the tropical stratosphere as well as in the extratropical stratosphere. For comparison, this will also be done using 4-D-Var analyses and 4-D-Var 3-day forecast series. An extra 4-D-Var 3-day forecast run is started in July, to study the dependence on season.

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4. Age-of-air calculation from five-year backward trajectories

The 5-year backward trajectories are started in the stratosphere on a global horizontal grid, with a resolution of $2^{\circ} \times 3^{\circ}$ latitude-longitude, i.e. 10 680 trajectories in total, at an altitude of 20 km. This horizontal resolution has been chosen to enable a comparison with the CTM age of air results obtained by Meijer et al. (2004), who used the same resolution. The altitude has been chosen to enable a comparison with the age observations by Andrews et al. (2001). All trajectories started at 56.23 hPa, being the geopotential height of 20 km in the US standard atmosphere. To reduce the amount of required ECMWF data, the 5-year trajectories are computed with data from only one year. The trajectories are started on 1 January 2001, 00:00 GMT and are integrated backward until 1 January 2000, 00:00 GMT. The resulting position is taken as start position for the next year's run with the same data.

Figure 3 shows, as a function of time, the fraction of trajectories that has reached the troposphere. The contribution to the mean age of each trajectory is weighted by the area of its starting grid cell. As motivated above, the three applied data sets are those used in the experiments 5, 6 and 8 of the sensitivity study (see Table 1). Hereafter these data sets will be denoted as, respectively, ERA40-FC1d, 4-D-Var-AN, and 4-D-Var-FC3d. After 5 years, for each of the three data sets more than 90% of the trajectories have reached the troposphere. The mean age of air for the ERA40-FC1d, the 4-D-Var-AN, and the 4-D-Var-FC3d data is, respectively, 1.36, 1.41, and 1.84 year (1.87 year for the 4-D-Var-FC3d July run). As follows from Eq. (2), the mean age is equal to the area between the vertical axis and the functional curve in Fig. 3; for ages larger than 5 years the curve has been extrapolated by applying an exponential fit, using the values at 3 and 5 year.

There is only a small sensitivity to the particular choice of 3 and 5 years. Using 2 years or 4 years instead of 3 years gave a difference of less than 1 day. Integrating till $T=4$ years, using 3 years and 4 years to estimate the mean age, gave a difference of only 5 days on a mean age of 672 days.

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The resulting mean age of air as a function of latitude for the ERA40-FC1d run and the 4-D-Var-AN run is shown in Fig. 4. The results of the corresponding runs with a CTM (Meijer et al., 2004) are also shown. Finally, the figure also shows the age of air derived from observations (Andrews et al., 2001).

In the CTM results the age in the extratropics of both hemispheres is larger for the 4-D-Var-AN than for the ERA40-FC1d data. In the trajectory results the age in the southern hemisphere is larger for the 4-D-Var-AN data, but in the northern hemisphere it is larger for the ERA40-FC1d data. Because the latter two differences nearly cancel, the ERA40-FC1d and 4-D-Var-AN trajectory-based global mean ages of air are, as mentioned above, almost the same. However, the trajectory runs seem to reproduce the gradient between the tropics and the mid-latitudes better.

In Fig. 5 the mean ages of all 4-D-Var runs are shown as a function of latitude. The 4-D-Var-FC3d ages are closest to the observations, but are still 0.5–1.5 year too small. For all data sets the computed age of air in the extratropics is smaller than observed. Compared to the difference in age between the results for the different data sets, the difference in age between the trajectory and the CTM results is small. We tentatively conclude that the sensitivity of the age of air in the CTM to the preprocessing is small. The effect of preprocessing might be largest near the equator, where the age in the CTM-results is larger than in the trajectory results, and even larger than observed.

5. Discussion and conclusions

This study was motivated by results from a chemistry transport model (CTM), driven by ECMWF data, in which the simulated age of stratospheric air was much smaller than observed. As the ECMWF data are preprocessed before they drive the model, the question arose to what extent this preprocessing influences the simulated age of air. A related question is whether the estimates of the age of air depend on the type of forecast series of the data, in particular the update frequency and the length of the forecasts series.

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We have chosen to integrate the trajectories for five years. By then, more than 90% of the trajectories had reached the troposphere (Fig. 3). For ages of more than five years we assumed an exponential fit with two parameters, which were determined from the observed values at two different times. The estimated mean age of air, based on a 4-year run, differed less than 1% from the result of the 5-year run.

We have not been able to estimate the uncertainty in the estimated age of air, because this would require a large number of multi-annual simulations, e.g. starting at different times, for which computational resources were not available. However, the latitudinal variability of the shown age estimates is expected to give a good impression of the uncertainty.

The results show that for the 3-D-Var ERA-40 data the age is largest for forecast series that are updated only once per day. However, this age is still smaller than the age obtained from any of the applied 4-D-Var data sets. For 4-D-Var data the age is largest for 3-day forecast series. This age, however, is still 0.5–1.5 year smaller than observed. We found that the difference between the age of air calculated with a CTM and a trajectory model, was small compared to the differences resulting from changes in the data set. Thus, the effect of preprocessing in the CTM on the age of air seems relatively small. Here it should be noted that quite some effort has gone into reducing numerical noise in the calculation of mass fluxes for the CTM from the data during preprocessing (Bregman et al., 2003)

We tested the sensitivity of the computed age of air to the precise definition of the tropopause. As an alternative to the potential temperature and potential vorticity-based definition mentioned in Sect. 2, we applied the traditional WMO definition involving a lapse-rate of 2 K/km. This changed the result for the global mean age of air by some 4%.

For the 5-year backward trajectory computations, the trajectories were all started in the northern winter season, on 1 January. This might lead to a bias in the computed age of air, because the stratospheric meridional circulation has a seasonal cycle, with strongest transport during northern winter. Thus, the number of trajectories leaving

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the stratosphere in the first months is expected to be relatively large, leading to an underestimation of the age of air. To investigate this effect, 5-year trajectories were computed, using 4-D-Var-FC3d data, with the same set-up as that for the other 5-year trajectories, but starting on 5 July. The computed mean age of air for these trajectories is 1.87 year, which is indeed slightly larger than the 1.84 year computed for the trajectories starting in January. As shown in Fig. 3, the larger age for the July-trajectories is mainly due to a decrease in the first months of the number of trajectories that reaches the troposphere. This is consistent with Fig. 5, which shows a higher age in the tropics for the July-trajectories.

We may conclude that the best choice to drive a CTM is using 4-D-Var data with a 3 day forecast series with timesteps 12 until 78. For the ERA-40 data set, applying a 1-day forecast series with timesteps 12 until 30 is the best choice.

Acknowledgements. The authors would like to acknowledge T. van Noije and B. Bregman for the inspiring discussions during our study.

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Table 1. Characteristics and results for the various data sets.

Exp.	Year	Source*	Forecast	Update	Grid	$F(50)^{**}$
1	1997	3-D-Var	6	6 h	1×1	46%
2	1997	3-D-Var	24, 30	12 h	1×1	22%
3	1997	3-D-Var	12, 18, 24, 30	24 h	1×1	15%
4	1997	3-D-Var	12, 18, 24, 30	24 h	2.5×2.5	14%
5	2000	3-D-Var	12, 18, 24, 30	24 h	3×2	16%
6	2000	4-D-Var	0	6 h	3×2	12%
7	2000	4-D-Var	12, 18, 24, 30	24 h	3×2	7%
8	2000	4-D-Var	12, 18,..., 78	3-Day	3×2	3%
9	2000	4-D-Var	18, 24, 30,..., 234	9 day	3×2	3%

* All input data are on 60 hybrid levels up to 0.1 hPa.

** $F(50)$ is the fraction (*100%) of the trajectories that has reached the troposphere at or before 50 days.

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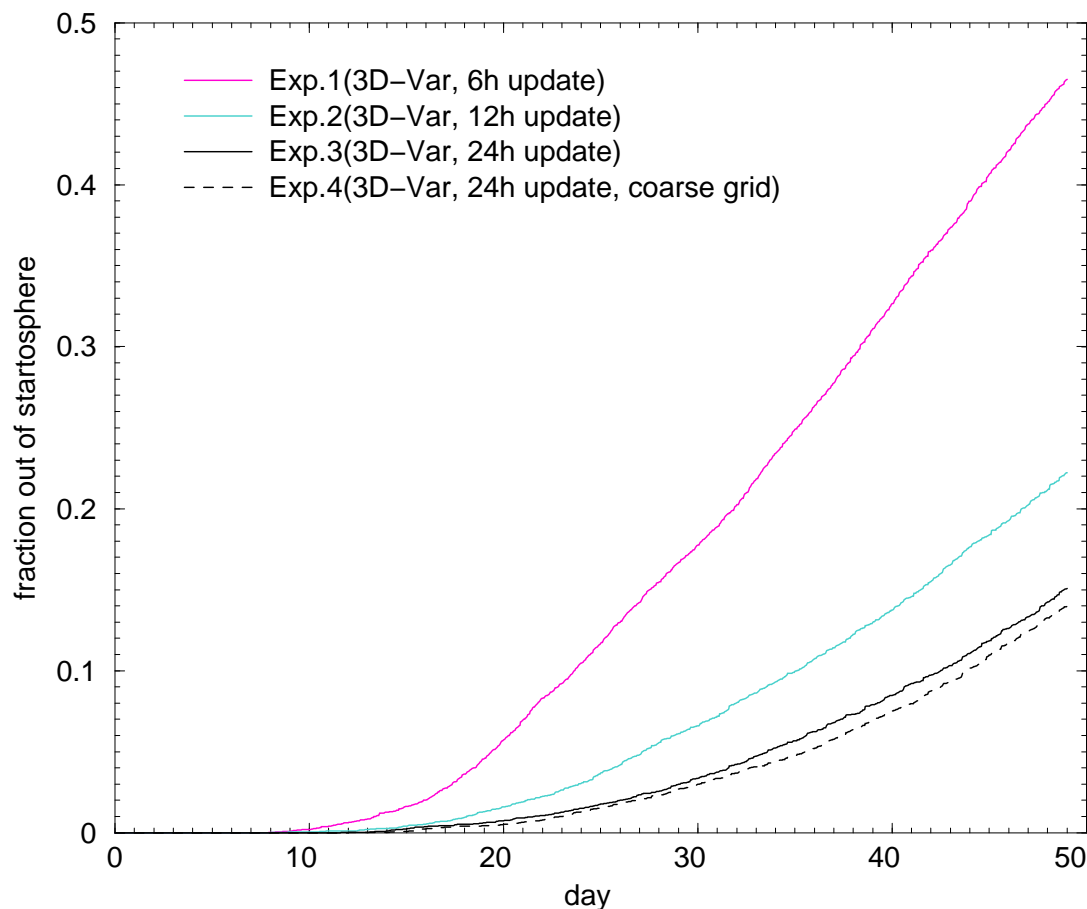


Fig. 1. The fraction of the 50-day-backward trajectories starting in the tropical lower stratosphere, that has reached the troposphere, as a function of time, for three different ERA-40 3-D-Var data sets, for 1997. The update frequencies are 6 h (Exp. 1), 12 h (Exp. 2) and 24 h (Exp. 3). Exp. 4 corresponds to Exp. 3 but has a coarser grid. See Table 1.

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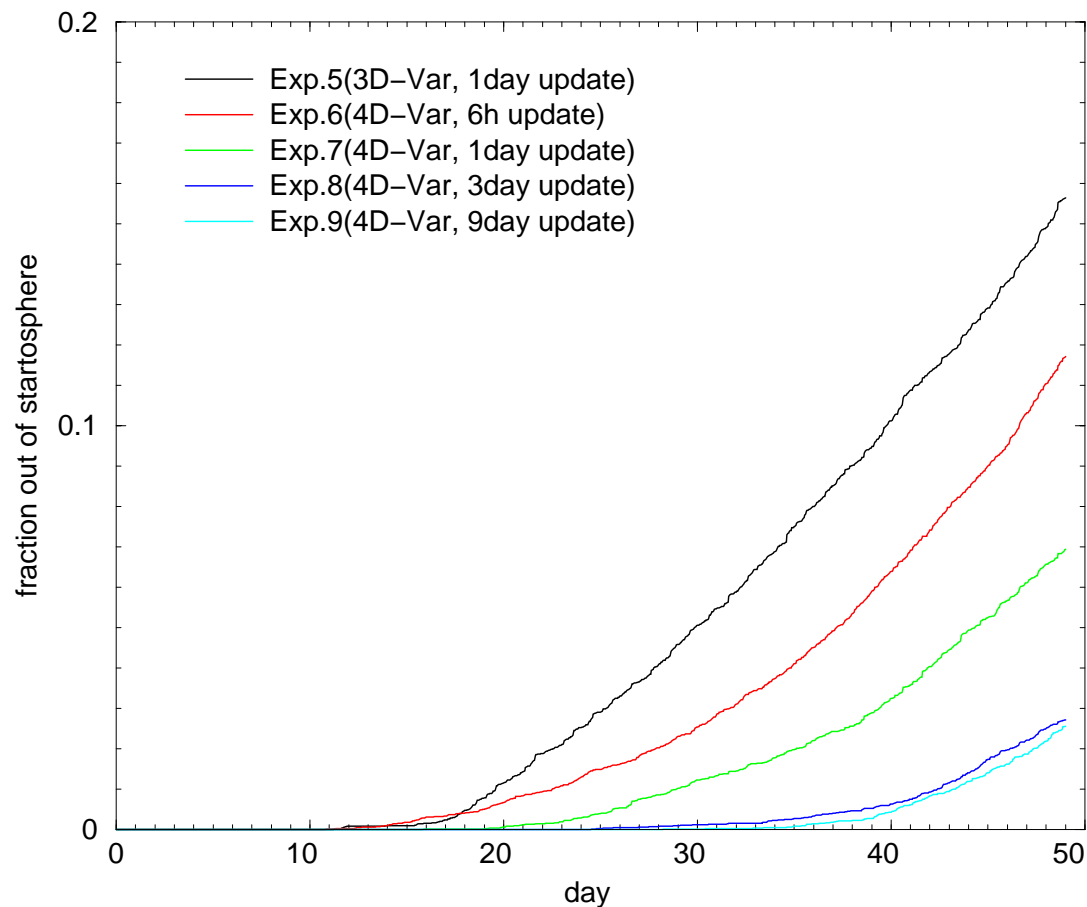


Fig. 2. As Fig. 1, but run for 2000 for one 3-D-Var ERA40 data set (Exp. 5) and four different 4-D-Var data sets. The update frequencies are 6 h (Exp. 6), 24 h (Exp. 5, 7), 3 day (Exp. 8) and 9 day (Exp. 9). See Table 1.

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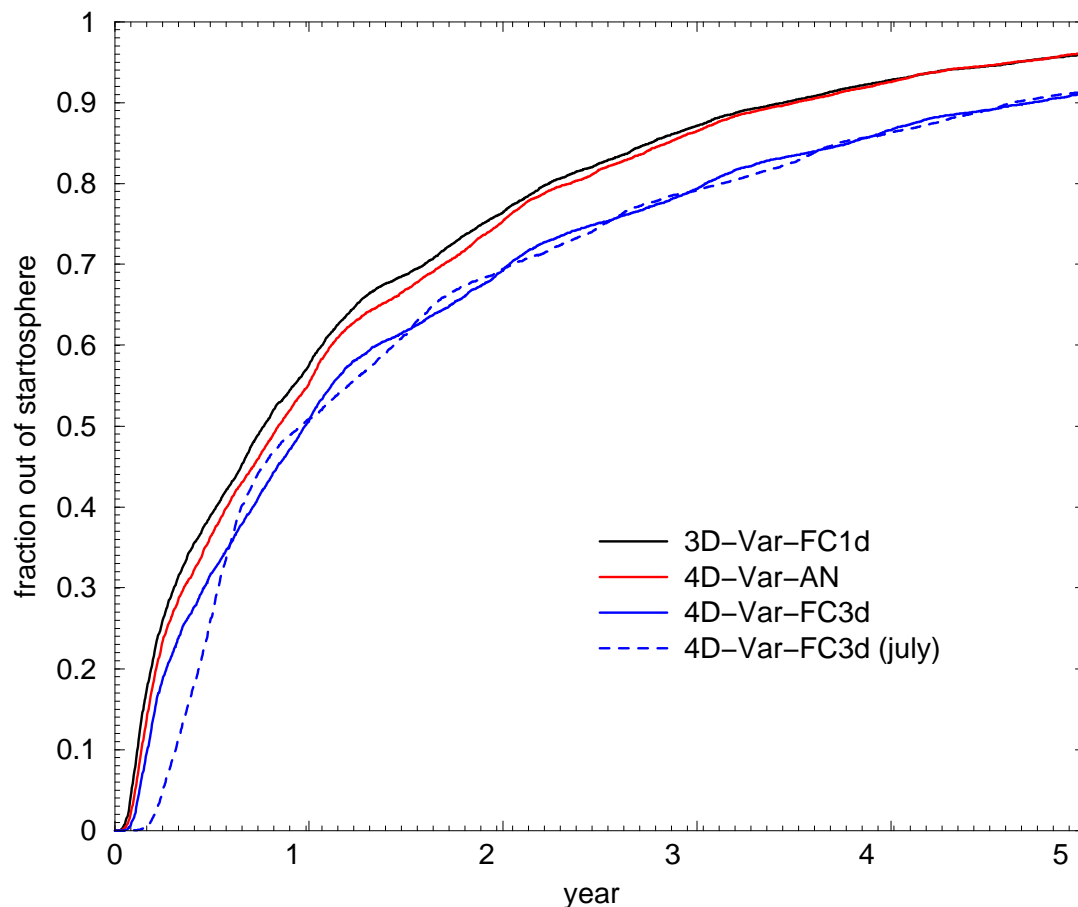


Fig. 3. The fraction of the 5-year-backward trajectories, starting at 20 km altitude, that has reached the troposphere, as a function of time, for 3-D-Var 1-day forecast series (3-D-Var-FC1d), 4-D-Var analyses (4-D-Var-AN), 4-D-Var 3 day-forecast series (4-D-Var-FC3d), and 4-D-Var 3 day-forecast series, starting in July (4-D-Var-FC3d(july)).

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Age of air at 20 km height

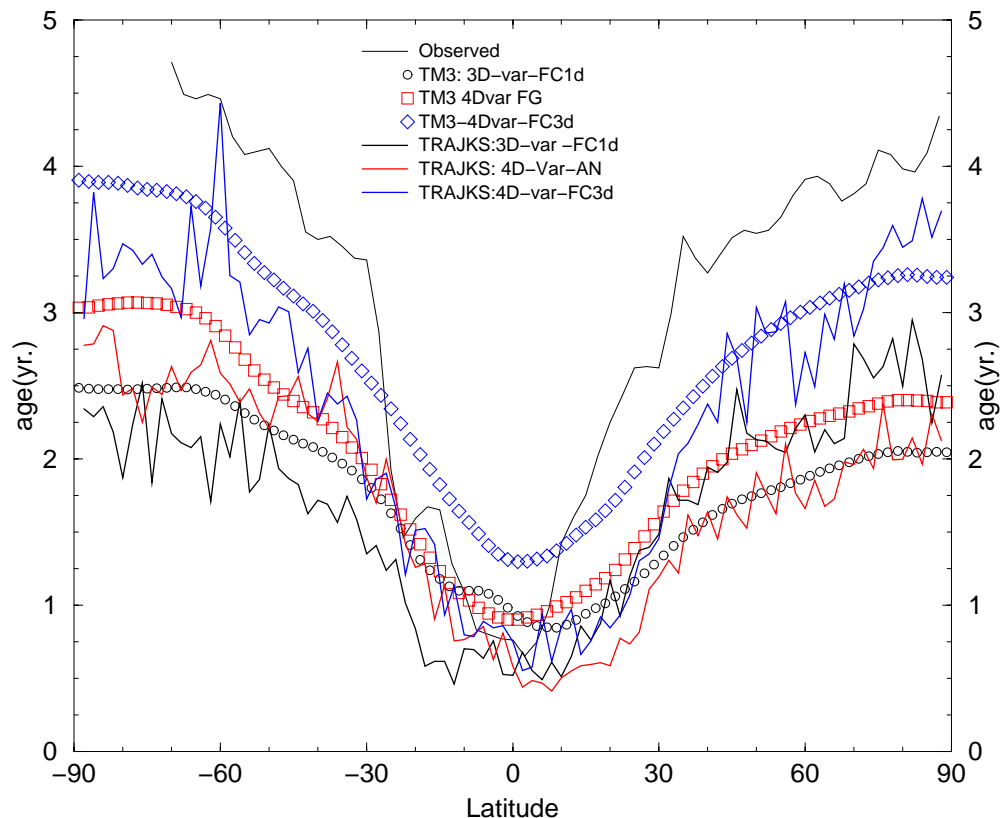


Fig. 4. The mean age of air, as a function of latitude, computed with the TRAJKS trajectory model and the TM3 CTM (Meijer et al., 2004), and as derived from observations (Andrews et al., 2001).

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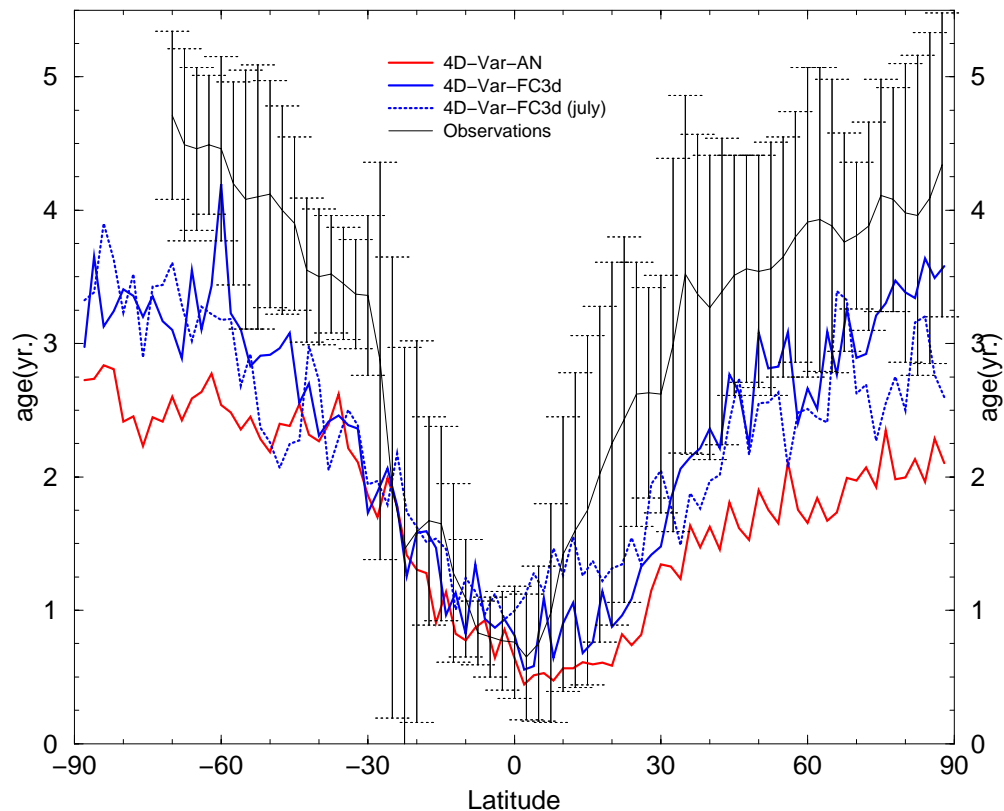


Fig. 5. The mean age of air, as a function of latitude, computed with the TRAJKS trajectory model with different data sets and as observed. The observation errors are marked in black.

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